2. SIMULATION MODELING

2.1 Temporal and Spatial Resolution and Numerical Stability

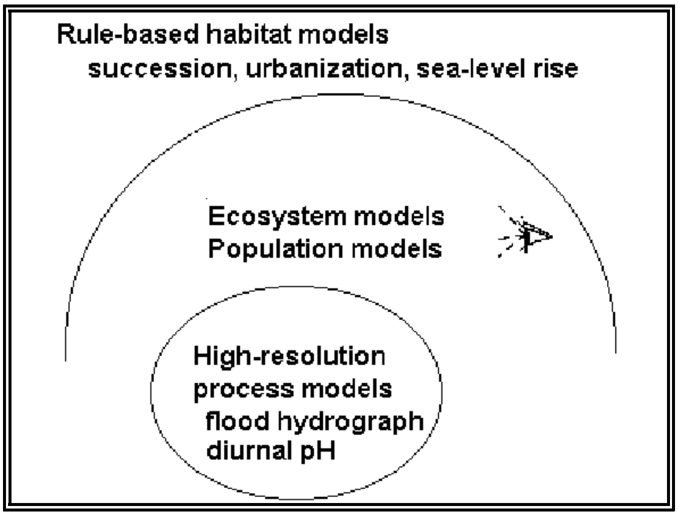
AQUATOX Release 1 is designed to be a general, realistic model of the fate and effects of pollutants in aquatic ecosystems. In order to be fast, easy to use, and verifiable, it has been designed with the simplest spatial and temporal resolutions consistent with this objective. It is designed to represent average daily conditions for a well-mixed aquatic system (in other words, a non-dimensional point model). It also can represent one-dimensional vertical epilimnetic and hypolimnetic conditions for those systems that exhibit stratification on a seasonal basis.

According to Ford and Thornton (1979), a one-dimensional model is appropriate for reservoirs that are between 0.5 and 10 km in length; if larger, then a two-dimensional model disaggregated along the long axis is indicated. The one-dimensional assumption is also appropriate for many lakes (Stefan and Fang, 1994). Similarly, one can consider a single reach or stretch of river at a time. A distributed version of the model (Version 2.00) is being developed; it will be able to simulate several linked stream reaches.

Usually the reporting time step is one day, but numerical instability is avoided by allowing the step size of the integration to vary to achieve a predetermined accuracy in the solution. This is a numerical approach, and the step size is not directly related to the temporal scale of the ecosystem simulation. AQUATOX uses a very efficient fourth- and fifth-order Runge-Kutta integration routine with adaptive step size to solve the differential equations (Press et al., 1986, 1992). The routine uses the fifth-order solution to determine the error associated with the fourth-order solution; it decreases the step size (often to 15 minutes or less) when rapid changes occur and increases the step size when there are slow changes, such as in winter. However, the step size is constrained to a maximum of one day so that short-term pollutant loadings are always detected.

The temporal and spatial resolution is in keeping with the generality and realism of the model (see Park and Collins, 1982). Careful consideration has been given to the hierarchical nature of the system. Hierarchy theory tells us that models should have resolutions appropriate to the objectives; phenomena with temporal and spatial scales that are significantly longer than those of interest should be treated as constants, and phenomena with much smaller temporal and spatial scales should be treated as steady-state properties or parameters (**Figure 3**, O'Neill et al., 1986). The model uses a longer time step than dynamic hydrologic models that are concerned with representing short-term phenomena such as storm hydrographs, and it uses a shorter time step than fate models that may be concerned only with long-term patterns such as bioaccumulation in large fish.

Figure 3. Position of Ecosystem Models such as AQUATOX in the Spatial-temporal Hierarchy of Models.



Changing the permissible relative error (the difference between the fourth- and fifth-order solutions) of the simulation can affect the results. The model allows the user to set the relative error, usually between 0.005 and 0.01. Comparison of output shows that up to a point a smaller error can yield a marked improvement in the simulation—although execution time is slightly longer. For example, simulations of two pulsed doses of chlorpyrifos in a pond exhibit a spread in the first pulse of about 0.6 μg/L dissolved toxicant between the simulation with 0.001 relative error and the simulation with 0.05 relative error (**Figure 4**); this is probably due in part to differences in the timing of the reporting step. However, if we examine the dissolved oxygen levels, which combine the effects of photosynthesis, decomposition, and reaeration, we find that there are pronounced differences over the entire simulation period. The simulations with 0.001 and 0.01 relative error give almost exactly the same results, suggesting that the more efficient 0.001 relative error should be used; the simulation with 0.05 relative error exhibits instability in the oxygen simulation; and the simulation with 0.1 error gives quite different values for dissolved oxygen (**Figure 5**). The observed mean daily maximum dissolved oxygen for that period was 9.2 mg/L (US EPA 1988), which corresponds most closely with the results of simulation with 0.001 and 0.01 relative error.

Figure 4. Pond with Chlorpyrifos in Dissolved Phase.

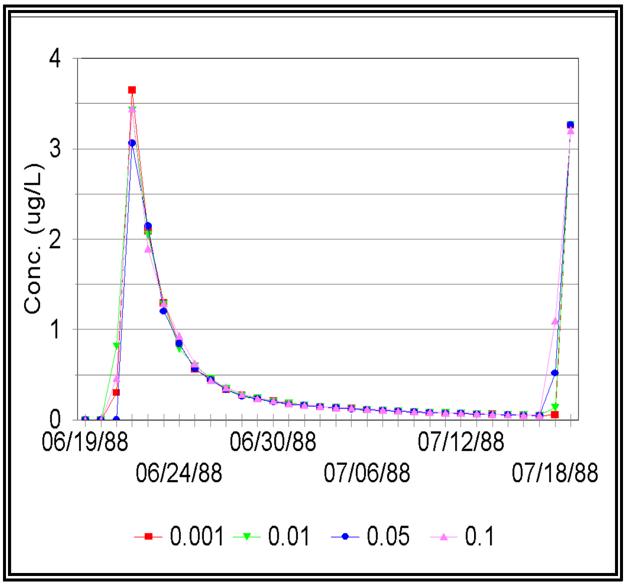
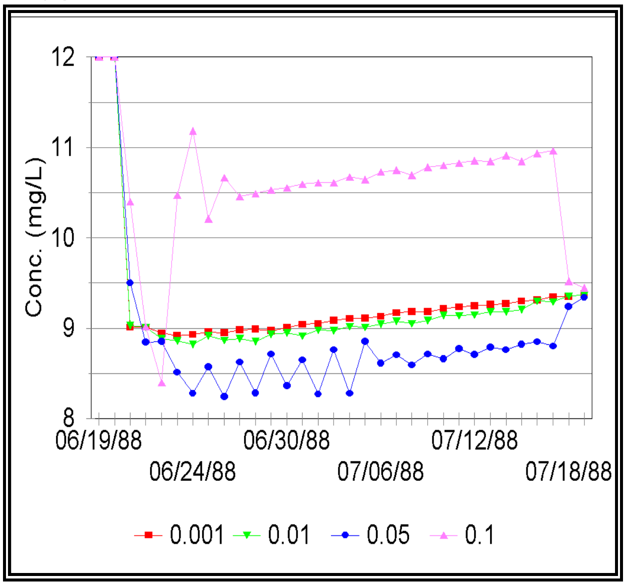


Figure 5. Same as **Figure 4** with Dissolved Oxygen.



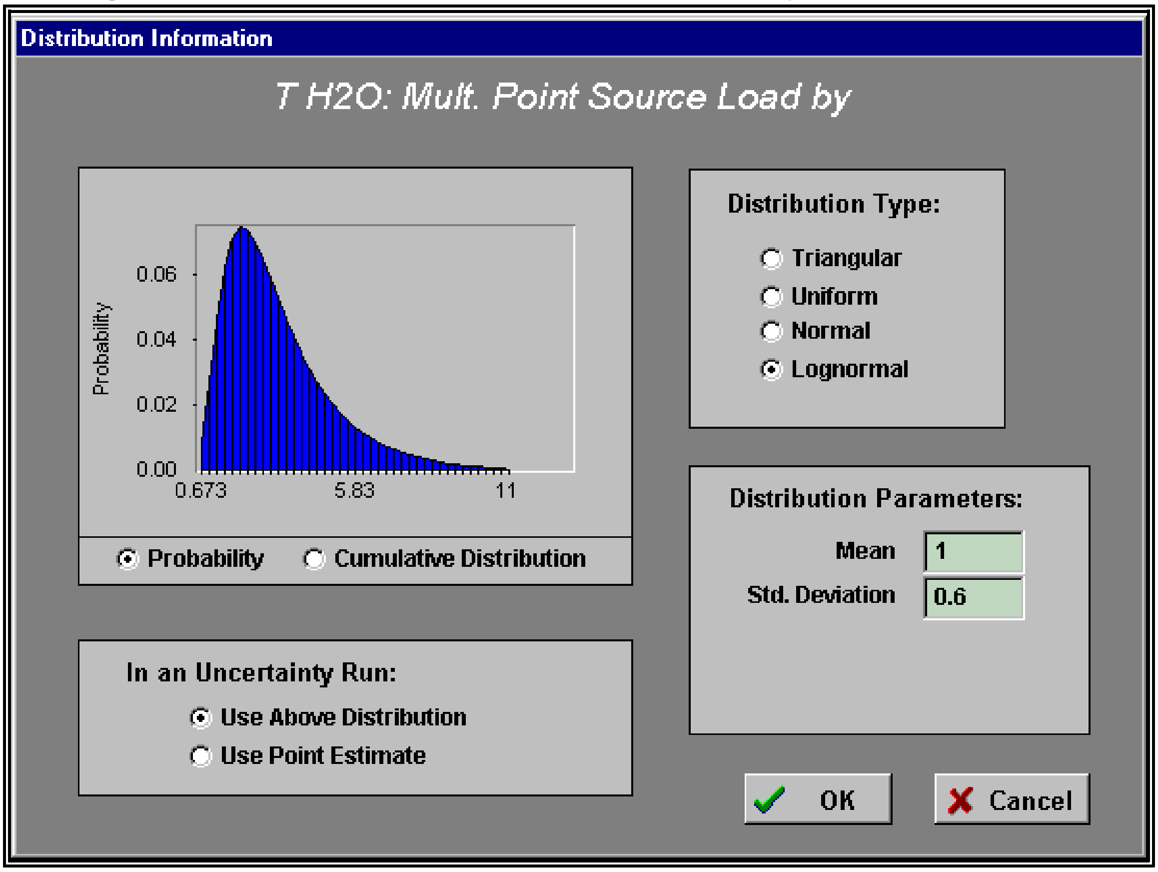
2.2 Uncertainty Analysis

There are numerous sources of uncertainty and variation in natural systems. These include: site characteristics such as water depth, which may vary seasonally and from site to site; environmental loadings such as water flow, temperature, and light, which may have a stochastic component; and critical biotic parameters such as maximum photosynthetic and consumption rates, which vary among experiments and representative organisms.

In addition, there are sources of uncertainty and variation with regard to pollutants, including: pollutant loadings from runoff, point sources, and atmospheric deposition, which may vary stochastically from day to day and year to year; physico-chemical characteristics such as octanol-water partition coefficients and Henry Law constants that cannot be measured easily; chemodynamic parameters such as microbial degradation, photolysis, and hydrolysis rates, which may be subject to both measurement errors and indeterminate environmental controls.

Increasingly, environmental analysts and decision makers are requiring probabilistic modeling approaches so that they can consider the implications of uncertainty in the analyses. AQUATOX provides this capability by allowing the user to specify the types of distribution and key statistics for a wide selection of input variables. Depending on the specific variable and the amount of available information, any one of several distributions may be most appropriate. A lognormal distribution is the default for environmental and pollutant loadings. In the uncertainty analysis, the distributions for constant loadings are sampled daily, providing day-to-day variation within the limits of the distribution, reflecting the stochastic nature of such loadings. Distributions for dynamic loadings may employ multiplicative factors that are sampled once each simulation (**Figure 6**). Normally the multiplicative factor for a loading is set to 1, but, as seen in the example, under extreme conditions the loading may be ten times as great. In this way the user could represent unexpected conditions such as pesticides being applied inadvertently just before each large storm of the season. Loadings usually exhibit a lognormal distribution, and that is suggested in these applications, unless there is information to the contrary.

Figure 6. Distribution Screen for Point-Source Loading of Toxicant in Water.



A sequence of increasingly informative distributions should be considered for most parameters (see **Volume 1: User's Manual**.) If only two values are known and nothing more can be assumed, the two values may be used as minimum and maximum values for a uniform distribution (**Figure 7**); this is often used for parameters where only two values are known. If minimal information is available but there is reason to accept a particular value as most likely, perhaps based on calibration, then a triangular distribution may be most suitable (**Figure 8**). Note that the minimum and maximum values for the distribution are constraints that have zero probability of occurrence. If additional data are available indicating both a central tendency and spread of response, such as parameters for well-studied processes, then a normal distribution may be most appropriate (**Figure 9**). The result of applying such a distribution in a simulation of Onondaga Lake, New York is shown in **Figure 10**, where simulated benthic feeding is seen to affect the sediment-water interaction and subsequently the predicted hypolimnetic anoxia. All distributions are truncated at zero because negative values would have no meaning. A non-random seed can be used for the random number generator, causing the same sequence of numbers to be picked in successive applications; this is useful if you want to be able to duplicate the results exactly.

Figure 7. Uniform Distribution for Henry's Law Constant for Esfenvalerate.

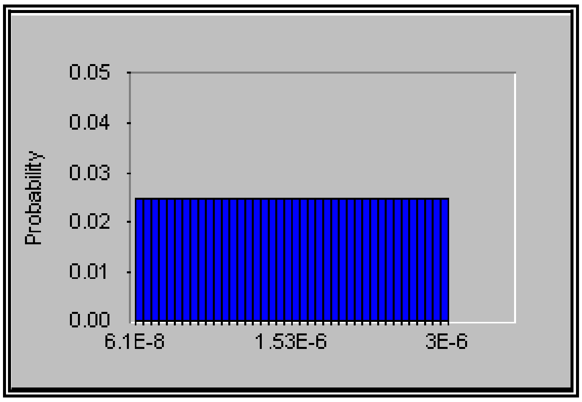


Figure 8. Triangular Distribution for Maximum Consumption Rate for Bass.

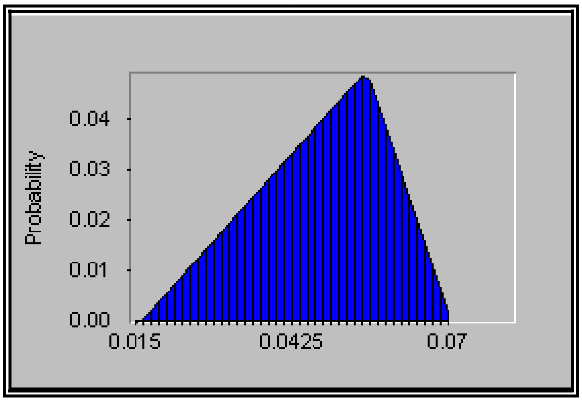
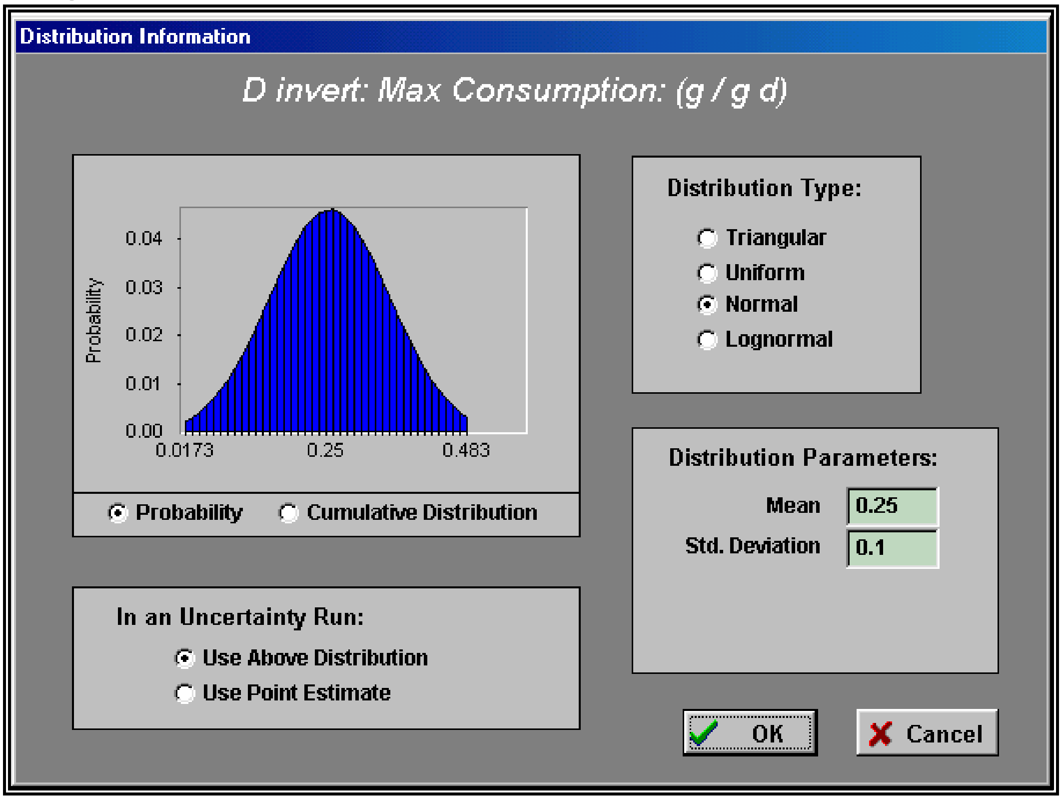


Figure 9. Normal Distribution for Maximum Consumption Rate for *Tubifex*.



Efficient sampling from the distributions is obtained with the Latin hypercube method (McKay et al., 1979; Palisade Corporation, 1991), using algorithms originally written in FORTRAN (Anonymous, 1988). Depending on how many iterations are chosen for the analysis, each cumulative distribution is subdivided into that many equal segments. Then a uniform random value is chosen *within* each segment and used in one of the subsequent simulation runs. For example, the distribution shown in **Figure 9** can be sampled as shown in **Figure 11**. This method is particularly advantageous because all regions of the distribution, including the tails, are sampled. The default is twenty iterations, meaning that twenty simulations will be performed with sampled input values; this should be considered the minimum number to provide any reliability. The optimal number can be determined experimentally by noting the number required to obtain convergence of mean response values for key state variables; in other words, at what point do additional iterations not result in significant changes in the results? As many variables may be represented by distributions as desired, but the method assumes that they are independently distributed. By varying one parameter at a time the sensitivity of the model to individual parameters can be determined. This is done for key parameters in the following documentation.

Figure 10. Sensitivity of Hypolimnetic Oxygen to Zoobenthic Feeding in Lake Onondaga New York.

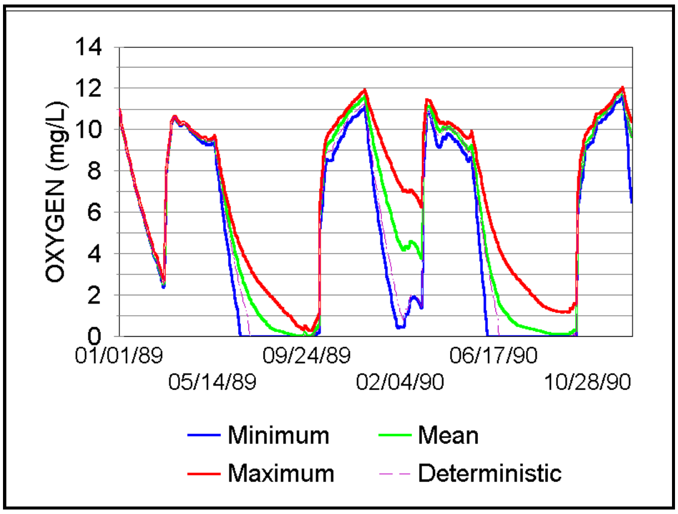


Figure 11. Latin Hypercube Sampling of a Cumulative Distribution with a Mean of 25 and Standard Deviation of 8 Divided into 5 Intervals.